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Computing the Determinant and the Algebraic Structure Count in Polygraphs

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An algorithm for computing the algebraic structure count in polygraphs is presented. It expresses the related determinant of the adjacency matrix of a polygraph in terms of the determinants of monographs and bonding edges between the monographs. The algorithm is illustrated on a class of polygraphs with two bonding edges between monographs and computations for selected examples of polygraphs of this class are presented.

Key words: determinant, algebraic structure count, polygraphs, acenylenes, phenylenes

INTRODUCTION

Perfect matchings of a molecular graph are known in chemistry as the Kekulé structures of the related molecule.[1–16] Kekulé and other valence bond structures have played for decades an important role in organic chemistry.[17]

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Especially, the stability of benzenoid hydrocarbons depends on the number K of Kekulé structures of the related hexagonal graphs. However, in the case of more general, but still alternant molecules (represented by bipartite graphs), the parity of Kekulé structures has to be taken into account in order to rationalize their stability.[5]

Two Kekulé structures are said to be of opposite (same) parity if one is obtained from the other by cyclically rearranging an even (odd) number of double bonds in a molecule. In this way, Kekulé structures decompose into two equivalence classes of opposite parity whose cardinalities are denoted by K_+ and K_-, where $K = K_+ + K_-$. The algebraic structure count, *ASC,* is then defined as:

$$ASC = | K_+ - K_- | \tag{1}$$

and it is able to model the stability of both benzenoid (where $ASC = K = K_+$) and other alternant molecules.[18,19] Similar quantity, Corrected Structure Count, was introduced by Herndon.[12,13]

In the present paper, we study *ASC* in polymers which are conveniently represented by polygraphs, especially those where building blocks of polymers are mutually isomorphic and where there is a uniform bonding between blocks. For such highly structured objects, efficient algorithms have been developed to compute various graph invariants. Many of them are based on extensive use of recursions for the invariant under consideration.[1,2,14,15] However, recursive formulae for the *ASC* depend in a complex manner on the structure of a graph (*cf.* Refs. 1 and 3). For several special classes like [*n*]acenylenes,[1,4] including their subclass of [*n*]phenylenes, circulenes,[10] antikekulene and its homologs,[9] recursive formulae have been obtained. However, one has to find some other route to compute the *ASC* in general. Fortunately, the *ASC* of a graph G can be expressed as:[7,8,17]

$$ASC^2 = | \det (\boldsymbol{A}) | \tag{2}$$

namely by the determinant of the adjacency matrix $\boldsymbol{A} = \boldsymbol{A}(\mathrm{G})$ of G, *i.e.*, by the constant coefficient of the characteristic polynomial of G.

Here we present an algorithm to compute the determinant of polygraphs as a new way to compute their *ASC*.

Let us note that the *ASC* loses its meaning in general, non-alternant molecules (represented by non-bipartite graphs) since the parity of their Kekulé structures can not be consistently defined. However, as the determinant of a graph has found applications in some chemical models (see, for example, Refs. 7 and 17), the method developed here could be of use in those models as well.

POLYGRAPHS

The notions of a monograph and a polygraph were introduced into chemical graph theory as a formalization of the chemical notions of monomer and polymer. Polygraphs with open (closed) ends are called fasciagraphs (rotagraphs) if all monographs are isomorphic and the bonding between them is uniform throughout a polygraph.

Let M_1, M_2, ..., M_n be arbitrary, mutually disjoint graphs, and let X_1, X_2, ..., X_n be a sequence of sets of unordered pairs of vertices such that $X_i \subseteq V(M_i) \times V(M_{i+1})$, i=1,2,..., n (where index i+1 is taken modulo n). Each pair $(x,y) \in X_i$ can be viewed as an edge joining the vertex x of $V(M_i)$ with a vertex y of $V(M_{i+1})$.

Observe that the edges in X_n join vertices of $V(M_n)$ with vertices of $V(M_1)$. A *polygraph*

$$\Omega_n = \Omega_n\ (M_1, M_2, ..., M_n; X_1, X_2, ..., X_n)$$

over *monographs* M_1, M_2, ..., M_n is defined in the following way:

$$V(\Omega_n) = V(M_1) \cup V(M_2) \cup ... \cup V(M_n),$$
$$E(\Omega_n) = E(M_1) \cup X_1 \cup E(M_2) \cup X_2 \cup ... \cup E(M_n) \cup X_n.$$

In the special case when M_1, M_2, ..., M_n are all isomorphic to a graph M (*i.e.*, all graphs M_i are disjoint copies of the monograph M) and $X_1 = X_2 = ... = X_n = X$, we call the polygraph a *rotagraph* and denote it by ω_n(M; X). A *fasciagraph* ψ_n(G; X) is defined similarly as a rotagraph ω_n(G; X) except that there are no edges between the first and the last copy of the monograph M, *i.e.*, $X_n = 0$. In the case of rotagraphs and fasciagraphs, we will consider their set of vertices as $V = \{1, ...,n\} \times V(M)$.

DETERMINANTS AND GRAPHS

The relationship between determinants and graphs is well established. Each term in the determinant A of the adjacency matrix $\boldsymbol{A} = \boldsymbol{A}(G)$ of a graph G is of the form $(-1)^{\mathrm{sgn}(\pi)}a_{1,\pi(1)}a_{2,\pi(2)}...a_{n,\pi(n)}$, where $n = |V(G)|$ and π is a permutation of $\{1,2,...,n\}$. The parity sgn(π) is a number of transpositions (modulo 2) needed to express π as their product. Any permutation can be written as a product of disjoint cyclic permutations. Each cyclic permutation corresponds to some directed cycle of G, and accordingly a permutation can be represented by a collection of pairwise disjoint directed cycles of various sizes (possibly including edges which are considered as cycles of length 2) which covers all vertices of G. Note that for permutations with at least one fixed point, their contribution to the determinant is 0 since the diagonal entries of $\boldsymbol{A}$ are equal to 0. (Therefore we may assume that there are no cycles of length 1.) It is easy to see that each directed cycle of even (odd) size in a collection contributes parity –1 (+1) and the total parity of a collection equals the product of parities of all directed cycles in a collection.

The above equivalence is illustrated in Figure 1 below for $G = C_4$ (the 4-membered cycle).

term in det A	$a_{12}a_{21}a_{34}a_{43}$	$a_{14}a_{23}a_{32}a_{41}$	$a_{12}a_{23}a_{34}a_{41}$	$a_{14}a_{21}a_{32}a_{43}$
permutation	(12) (34)	(14) (23)	(1234)	(1432)
parity	(-1) (-1) = +1	(-1) (-1) = +1	(-1)	(-1)

collection of directed cycles

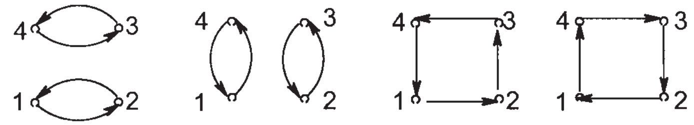

Figure 1. Representation of permutations by collections of directed cycles in C_4.

Therefore, the value of $\det(\boldsymbol{A}(C_4))$ equals +1+1–1–1 = 0.

The above considerations give a general answer on the dependence of $\det(\boldsymbol{A}(G)) = \det(G)$ on the structure of a graph G: see, for example, Refs. 11 and 7.

$$\det(G) = \sum_{H} (-1)^{C_{even}(H)} \tag{3}$$

where the summation is taken over all collections H of pairwise disjoint directed cycles of G and $C_{even}(H)$ stands for the number of directed cycles of even size (length) in H.

Let us note that, although the graphs used in chemistry are undirected, it is easy to represent them by equivalent directed graphs simply by replacing every edge of G by a pair of oppositely directed arcs.

METHOD

In order to develop a recursion formula to compute *ASC* of polygraphs, we need a generalization of formula (3). Consider a polygraph $\Omega_n = \Omega_n(M_1, M_2, ..., M_n; X_1, X_2, ..., X_n)$. In order to simplify the arguments, let us first consider a polygraph $G_2 = \Psi_2(M_1, M_2; X_1, X_2)$ depicted in Figure 2 where X_1

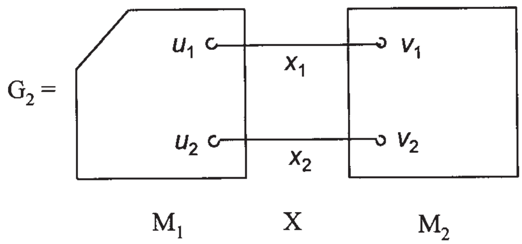

Figure 2. Polygraph with open ends having two monographs joined by two edges.

= X = $\{x_1, x_2\}$, $X_2 = \emptyset$, *i.e.*, a polygraph with *open* ends obtained from two monographs M_1 and M_2 joined by only two edges $x_1 = u_1v_1$ and $x_2 = u_2v_2$.

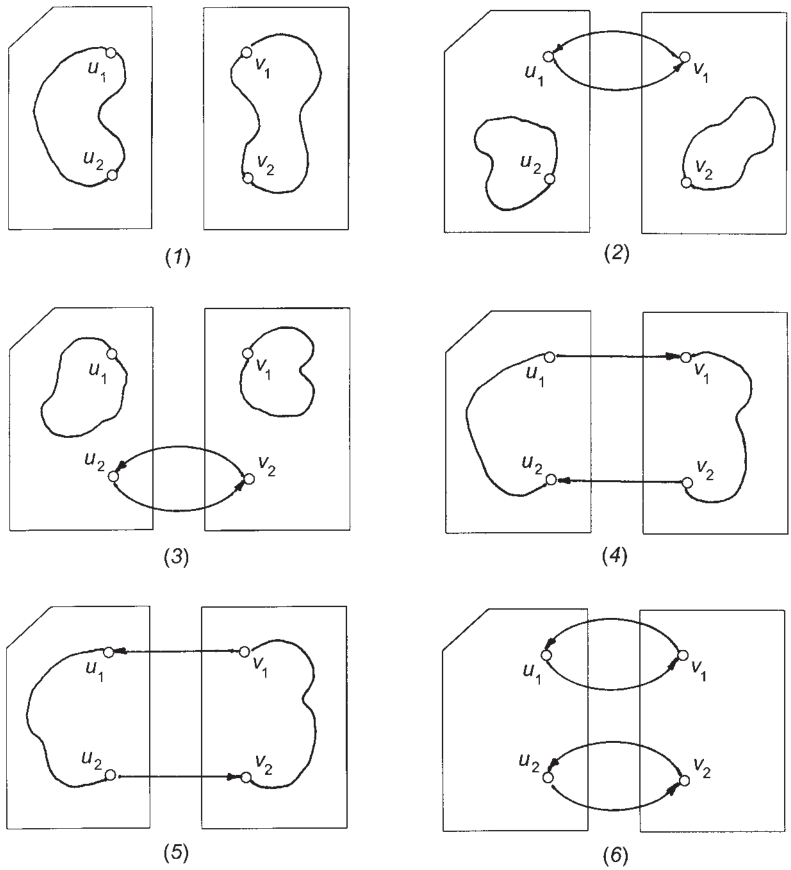

Figure 3. Six types of directed cycles in G_2 contributing to det (G_2).

In order to compute det(G_2), one has to consider all collections of directed cycles in G_2. Each directed cycle in G_2 is either completely contained in M_1 or M_2 or it contains the arcs of X together with some arcs of M_1 and M_2. All possible contributions to det(G_2) are shown in Figure 3 where, in order to keep the drawings simple, only directed cycles containing vertices u_1, u_2, v_1, v_2 are depicted.

There are altogether six various types of contributions (called types (*1*)–(*6*) as denoted in Figure 3). Contributions of type (*1*) correspond to collections of all directed cycles completely in M_1 and M_2. It is easy to see that the contributions of all such collections of cycles in (3) contribute to det(G_2) precisely the value equal to

$$\det(M_1)\ \det(M_2). \tag{4}$$

The contributions of type (*2*) correspond to collections of directed cycles in M_1 and M_2 such that one of the cycles is the 2-membered cycle with vertices u_1 and v_1. They contribute to det(G_2) the value which is equal to

$$-\det(M_1 - u_1)\ \det(M_2 - v_2) \tag{5}$$

where –1 comes from the parity of the 2-membered cycle u_1v_1. A similar argument holds for contributions of type (*3*).

For contributions of type (*4*) we replace each directed cycle by two directed cycles, as shown in Figure 4, where each of u_1u_2 and v_2v_1 is just on edge add to the graph.

If the length of the original cycle is d, then we get two cycles of lengths d_1 and d_2, respectively, where $d_1 + d_2 = d$. Obviously, the number of even cycles is 0 or 2 if d is even, and it is equal to 1 if d is odd. In both cases, the number of even cycles changes its parity.

The above construction can be formulated in terms of determinants as follows: in the adjacency matrix of M_1, replace the row of u_1 by a row of zeros, the column of u_2 by a column of zeros, and put matrix element equal to 1 in position u_1u_2. Denote such matrix by $(M_1)_{out=u_1}^{in=u_2}$. In terms of the graph, this construction corresponds to deletion of all arcs emanating (outgoing) from vertex u_1 to other vertices, deletion of all arcs sinking (ingoing) at vertex u_2, and addition of arc u_1u_2. Therefore, the corresponding contribution to the determinant can be written as

$$-\det\left((M_1)_{out=u_1}^{in=u_2}\right) \det\left((M_2)_{out=v_2}^{in=v_1}\right), \tag{6}$$

where the minus sign is due to the change of parity of the number of even cycles. Similar procedure applies to contributions of type (*5*) and they contribute to det(G_2) a value given by

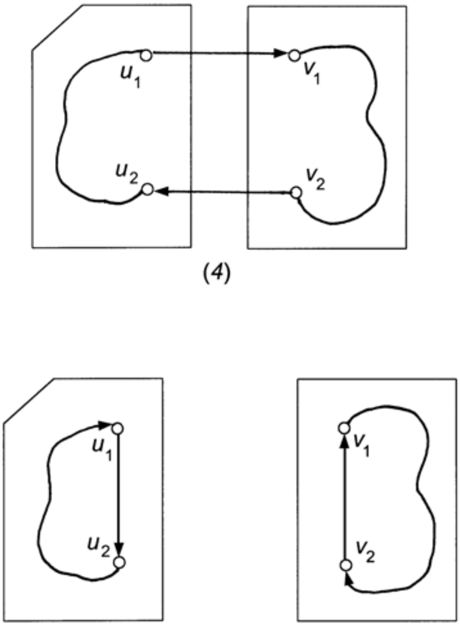

Figure 4. Replacement of directed cycle belonging to contribution *(4)* by two directed cycles.

$$-\det\big((\mathrm{M}_1)^{in=u_1}_{out=u_2}\big)\,\det\big((\mathrm{M}_2)^{in=v_2}_{out=v_1}\big). \tag{7}$$

Similarly, contributions of type (*6*) add to $\det(\mathrm{G}_2)$ a value of

$$\det(\mathrm{M}_1–u_1–u_2)\ \det(\mathrm{M}_2–v_1–v_2). \tag{8}$$

The sum of all above terms can be conveniently written in matrix form as:

$$\det(\mathrm{G}_2) = \boldsymbol{A}^{(1)}\,\boldsymbol{X}\,(\boldsymbol{A}^{(2)})^T\ . \tag{9}$$

The row vector $\boldsymbol{A}^{(1)}$ picks up the left factors of the contributions discussed above:

$$\boldsymbol{A}^{(1)} = \big((\det(\mathrm{M}_1),\ \det(\mathrm{M}_1–u_1),\ \det(\mathrm{M}_1–u_2),$$
$$\det(\mathrm{M}_1)^{in=u_2}_{out=u_1},\ \det(\mathrm{M}_1)^{in=u_1}_{out=u_2},\ \det(\mathrm{M}_1–u_1–u_2)\big). \tag{10}$$

The matrix $\boldsymbol{X}$ is equal to:

$$
\boldsymbol{X} = \begin{array}{c} \\ (1) \\ (2) \\ (3) \\ (4) \\ (5) \\ (6) \end{array}
\begin{array}{c} \begin{array}{cccccc} \mathit{1} & \mathit{2} & \mathit{3} & \mathit{4} & \mathit{5} & \mathit{6} \end{array} \\
\begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix} \end{array}
$$

The column vector $(\boldsymbol{A}^{(2)})^T$ takes care of the right factors in the above contributions and is given by:

$$
\boldsymbol{A}^{(2)} = \Big(\det(\mathrm{M}_2),\ \det(\mathrm{M}_2 - v_1),\ \det(\mathrm{M}_2 - v_2),
$$

$$
\det((\mathrm{M}_2)^{in=v_1}_{out=v_2},\ \det((\mathrm{M}_2)^{in=v_2}_{out=v_1},\ \det(\mathrm{M}_2 - v_1 - v_2)\Big)\ . \tag{11}
$$

Note that a given ordering of contributions depicted in Figure 3 induces indexing in (row and column) vectors and matrix $\boldsymbol{X}$. Once an ordering is chosen, it has to be fixed throughout the computations.

Let us now consider a general polygraph $\Psi_n = \Psi_n(\mathrm{M}_1, \mathrm{M}_2, \ldots, \mathrm{M}_n; \mathrm{X}_1, \mathrm{X}_2, \ldots, \mathrm{X}_n)$ with *open* ends (*i.e.*, X_n=0). For $\det(\Psi_n)$ one deduces:

$$
\det(\Psi_n) = \boldsymbol{A}^{(1)}\boldsymbol{X}^{(1)}\ \boldsymbol{A}^{(2)}\boldsymbol{X}^{(2)},\ \ldots,\ \boldsymbol{X}^{(n-1)}(\boldsymbol{A}^{(n)})^T \tag{12}
$$

where matrices $\boldsymbol{X}^{(1)}, \boldsymbol{X}^{(2)}, \ldots, \boldsymbol{X}^{(n-1)}$ are constructed in analogy with $\boldsymbol{X}$. The row vectors $\boldsymbol{A}^{(1)}$ and $\boldsymbol{A}^{(n)}$ related to the leftmost and rightmost monographs of Ψ_n are constructed in the same way as vectors $\boldsymbol{A}^{(1)}$ and $\boldsymbol{A}^{(2)}$. However, $\boldsymbol{A}^{(2)}$, $\boldsymbol{A}^{(3)}, \ldots, \boldsymbol{A}^{(n-1)}$ become matrices. *E.g.*, matrix $\boldsymbol{A}^{(i)}$ is a rectangular $\boldsymbol{S}^1 \times \boldsymbol{S}^2$ matrix where $\boldsymbol{S}^1$ and $\boldsymbol{S}^2$ are equal to the number of all possible types of contributions defined on the set of edges X_{i-1} and X_i, respectively.

The above formulae for the determinant of a polygraph take a simpler form if one deals with regular polygraphs, in which case, due to the isomorphism of all monographs and uniformity of all sets of connecting edges, one has:

$$
\boldsymbol{A} = \boldsymbol{A}^{(2)} = \ldots = \boldsymbol{A}^{(n-1)},\ \boldsymbol{X} = \boldsymbol{X}^{(1)} = \boldsymbol{X}^{(2)} = \ldots = \boldsymbol{X}^{(n-1)}. \tag{13}
$$

Therefore the determinants of fasciagraphs are given by:

$$
\det(\psi_n) = \boldsymbol{A}^{(1)}\ (\boldsymbol{X}\ \boldsymbol{A})^{n-2}\ \boldsymbol{X}\ (\boldsymbol{A}^{(n)})^T\ . \tag{14}
$$

EXAMPLES

We shall illustrate the method developed in this paper on a class of graphs describing [n]phenylenes, a class of molecules that have recently attracted a considerable attention among chemists; see Ref. 1 and references therein.

[n]phenylenes are polycyclic conjugated molecules composed of n 6-membered rings that are coupled to each other *via* cyclobutadiene (4-membered ring) units. [n]acenylenes are a generalization of these molecules where a single hexagon is replaced by h fused hexagons (polyacene). (Thus [n]phenylenes can be viewed as a special case where h=1.) Fusion could be done in a linear, spiral and zig-zag manner, thus defining the fasciagraphs X_n, Y_n and Z_n, respectively, shown in Figure 5. The index n denotes the number of monographs. In all these classes, monographs are the same (for a given value of h).

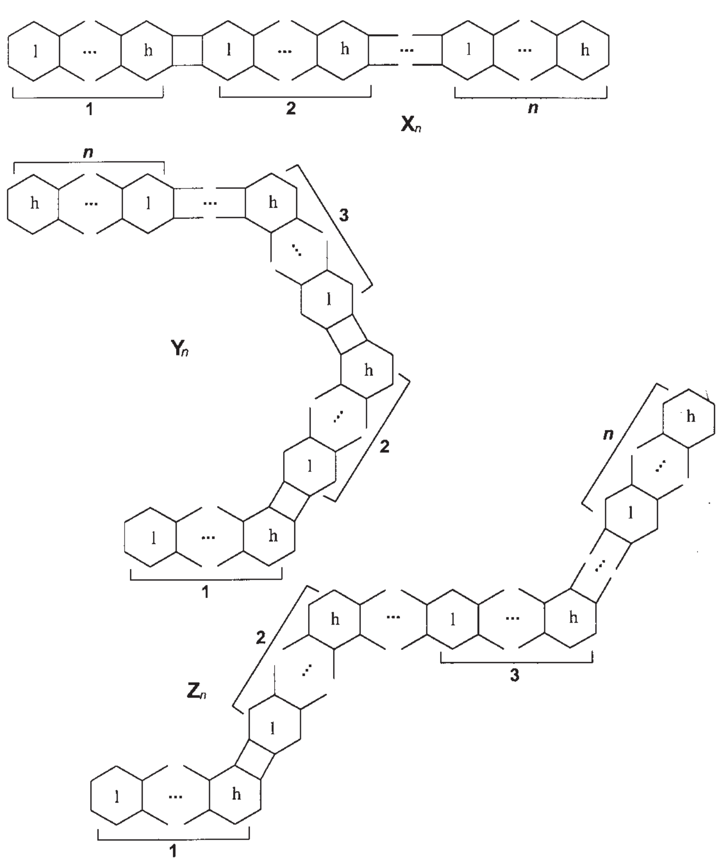

Figure 5. Linear (X_n), spiral (Y_n) and zig-zag (Z_n [n]acenylenes.

Note that in all these fasciagraphs the monographs are connected by two edges only, and one meets the case elaborated above in full detail. Recall that there were exactly six various types of contributions. In the following examples, we adopt the same ordering of contributions and indexing of vectors and matrices as given before.

Example 1. For linear fasciagraphs X_n with h = 1, one has:

$$\boldsymbol{A}^{(1)} = [-4,0,2,2,0,1],\ \boldsymbol{A}^{(2)} = [-4,0,2,2,0,1],$$

$$\boldsymbol{X} = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix}, \qquad \boldsymbol{A} = \begin{bmatrix} -4 & 0 & 2 & 2 & 0 & 1 \\ 0 & 0 & 0 & 0 & -1 & 0 \\ 2 & 0 & -1 & 0 & 0 & 0 \\ 2 & 0 & 0 & -1 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 \end{bmatrix},$$

$$\boldsymbol{A} \cdot \boldsymbol{X} = \begin{bmatrix} -4 & 0 & 2 & 2 & 0 & 1 \\ 0 & 0 & 0 & 0 & -1 & 0 \\ 2 & 0 & -1 & 0 & 0 & 0 \\ 2 & 0 & 0 & -1 & 0 & 0 \\ 0 & -1 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

and $\det(X_n)$ and $ASC(X_n)$ can be calculated by Eq. (14). For n = 1, 2, ..., 20, the results are assembled below:

n	$\det(X_n)$	$ASC(X_n)$	n	$\det(X_n)$	$ASC(X_n)$
1	–4	2	11	–144	12
2	9	3	12	169	13
3	–16	4	13	–196	14
4	25	5	14	225	15
5	–36	6	15	–256	16
6	49	7	16	289	17
7	–64	8	17	–324	18
8	81	9	18	361	19
9	–100	10	19	–400	20
10	121	11	20	441	21

Example 2. For spiral fasciagraphs Y_n with $h = 1$, $\boldsymbol{A}^{(1)}$, $\boldsymbol{A}^{(2)}$, $\boldsymbol{X}$ are as in the previous example, while:

$$\boldsymbol{A}=\begin{bmatrix} -4 & 0 & 2 & 2 & 0 & 1 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 2 & 0 & -1 & -2 & 0 & -1 \\ 2 & 0 & -2 & -1 & 0 & -1 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 1 & 0 & -1 & -1 & 0 & -1 \end{bmatrix}, \qquad \boldsymbol{A}\cdot\boldsymbol{X}=\begin{bmatrix} -4 & 0 & -2 & -2 & 0 & 1 \\ 0 & -1 & 0 & 0 & 0 & 0 \\ 2 & 0 & 1 & 2 & 0 & -1 \\ 2 & 0 & 2 & 1 & 0 & -1 \\ 0 & 0 & 0 & 0 & -1 & 0 \\ 1 & 0 & -1 & 1 & 0 & -1 \end{bmatrix}$$

and for $n = 1, 2, ..., 20$, one obtains:

n	det(X_n)	*ASC*(X_n)	n	det(X_n)	*ASC*(X_n)
1	–4	2	11	–54289	233
2	9	3	12	142129	377
3	–25	5	13	–372100	610
4	64	8	14	974169	987
5	–169	13	15	–2550409	1597
6	441	21	16	6677056	2584
7	–1156	34	17	–17480761	4181
8	3025	55	18	45765225	6765
9	–7921	89	19	–119814916	10946
10	20736	144	20	313679521	17711

Example 3. In the case of zig-zag fasciagraphs Z_n with $h = 1$, $\boldsymbol{A}^{(1)}$, $\boldsymbol{A}^{(2)}$, $\boldsymbol{X}$ are the same as in the previous example, and it appears convenient to take two consecutive monographs as a new monograph, M', whose related matrices are given by

$$\boldsymbol{A}'=\begin{bmatrix} 9 & 0 & -3 & -3 & 0 & -1 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ -3 & 0 & 1 & 0 & 0 & 0 \\ -3 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ -1 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}, \qquad \boldsymbol{A}'\cdot\boldsymbol{X}=\begin{bmatrix} 9 & 0 & 3 & 3 & 0 & -1 \\ 0 & -1 & 0 & 0 & 0 & 0 \\ -3 & 0 & -1 & 0 & 0 & 0 \\ -3 & 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 & -1 & 0 \\ -1 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

One should distinguish between the even and odd values of n.

For even $n = 2k$: $\det(Z_n) = \boldsymbol{A}^{(1)}\, \boldsymbol{X}\, (\boldsymbol{A}'\, \boldsymbol{X})^{k-1}\, (\boldsymbol{A}^{(2)})^T$, and for $n = 2, 4, \ldots, 20$ one gets:

n	$\det(Z_n)$	$ASC(Z_n)$	n	$\det(Z_n)$	$ASC(Z_n)$
2	9	3	12	142129	377
4	64	8	14	974169	987
6	441	21	16	6677056	2584
8	3025	55	18	45765225	6765
10	20736	144	20	313679521	17711

For odd $n = 2k+1$, by taking into account one more monograph at the end, $\boldsymbol{A}^{(2)}$ should be replaced by vector $\boldsymbol{A}' = [-4,0,2,2,0,1]$. Now one has: $\det(Z_{2k+1}) = \boldsymbol{A}^{(1)} \cdot \boldsymbol{X} \cdot (\boldsymbol{A} \cdot \boldsymbol{X})^{k-2} \cdot (\boldsymbol{A}')^T$, and thus for $n=1, 3, \ldots, 19$, one gets:

n	$\det(Z_n)$	$ASC(Z_n)$	n	$\det(Z_n)$	$ASC(Z_n)$
1	–4	2	11	–54289	233
3	–25	5	13	–372100	610
5	–169	13	15	–2550409	1597
7	–1156	34	17	–17480761	4181
9	–7921	89	19	–119814916	10946

Example 4. For linear acenylenes X_n with $h=2$, one has:

$$\boldsymbol{A}^{(1)} = [-9,0,3,3,0,1],\ \boldsymbol{A}^{(2)} = \boldsymbol{A}^{(1)},$$

$$\boldsymbol{A} = \begin{bmatrix} -9 & 0 & 3 & 3 & 0 & 1 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 3 & 0 & -1 & 0 & 0 & 0 \\ 3 & 0 & 0 & -1 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}, \qquad \boldsymbol{A} \cdot \boldsymbol{X} = \begin{bmatrix} -9 & 0 & -3 & -3 & 0 & 1 \\ 0 & 0 & 0 & 0 & -1 & 0 \\ 3 & 0 & 1 & 0 & 0 & 0 \\ 3 & 0 & 0 & 1 & 0 & 0 \\ 0 & -1 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

and, accordingly, for $n=1, 2, \ldots, 20$, one obtains:

n	$\det(X_n)$	$ASC(X_n)$	n	$\det(X_n)$	$ASC(X_n)$
1	–9	3	11	–2149991424	46368
2	64	8	12	14736260449	121393
3	–441	21	13	–101003831721	317811
4	3025	55	14	692290561600	832040
5	–20736	144	15	–4745030099481	2178309
6	142129	377	16	32522920134769	5702887
7	–974169	987	17	–222915410843904	14930352
8	6677056	2584	18	1527884955772561	39088169
9	–45765225	6765	19	–10472279279564025	102334155
10	313679521	17711	20	71778070001175616	267914296

It turns out that the recursion for determinants is given by: $a_n = -7\, a_{n-1} - a_{n-2} + 2(-1)^n$, while for the *ASC* by: $a_n = 3\, a_{n-1} - a_{n-2}$.

The recursions for the determinants and the *ASC* of Examples 1–3 can be found in Ref. 1.

Example 5. For spiral acenylenes Y_n with h=2, one has:

$$\boldsymbol{A}^{(1)} = [-9,0,3,3,0,1],\ \boldsymbol{A}^{(2)} = \boldsymbol{A}^{(1)},$$

$$\boldsymbol{A} = \begin{bmatrix} -9 & 0 & 3 & 3 & 0 & 1 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 6 & 0 & -2 & -3 & 0 & -1 \\ 6 & 0 & -3 & -2 & 0 & -1 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 4 & 0 & -2 & -2 & 0 & -1 \end{bmatrix}$$

and for n=1, 2, ..., 20, one obtains:

n	det(Y_n)	*ASC*(Y_n)	n	det(Y_n)	*ASC*(Y_n)
1	–9	3	11	–277089316	16646
2	49	7	12	1614994969	40187
3	–196	14	13	–9412880400	97020
4	225	35	14	54862287529	234227
5	–7056	84	15	–319760844676	565474
6	41209	203	16	1863702780625	1365175
7	–240100	490	17	–10862455838976	3295824
8	1399489	1183	18	63311032253329	7956823
9	–8156736	2856	19	–369003737680900	19209470
10	47541025	6895	20	2150711393832169	46375763

The recursion for determinants is given by: $a_n = -6\, a_{n-1} - a_{n-2} + 98$, and for *ASC* by: $a_n = 2\, a_{n-1} + a_{n-2}$. This recursion as well as recursive formulae for some other cases of Examples 1–5 were calculated in Ref. 1.

CONCLUSIONS

The difficult problem of computing the *ASC* in polygraphs has been reduced here to computation of the determinant (of the adjacency matrix) of polygraphs. This determinant has been calculated as the appropriate product of matrices $\boldsymbol{A}$, $\boldsymbol{X}$ and row (column) vectors which describe monographs, linking edges situation and (in the case of polygraphs with open ends) the leftmost (rightmost) monograph, respectively. Although only polygraphs with two linking edges between monographs are treated here in full detail, the algorithm can be generalized to polygraphs with more linking edges. The Laplace expansion of determinant over more rows and columns (see, Ref. 16, p. 106, and Ref. 6, p. 36) and its graphical representation should be of use in such generalizations.

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SAŽETAK

Računanje determinante i broja algebarskih struktura u poligrafovima

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Prikazan je algoritam za računanje broja algebarskih struktura u poligrafovima, u kojemu se pripadna determinanta matrice susjedstva poligrafa izražava preko determinanti monografova i veza među monografovima. Za ilustraciju algoritma poslužila je klasa poligrafova u kojima su monografovi međusobno povezani sa dvije veze. Prikazani su rezultati računa za više poligrafova te klase.